Physics Through Problem Solving XXVI: Variational Method

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Abstract

In this issue we shall illustrate the variational method of estimating the ground state energy of a quantum mechanical system.

We obtain the energy eigenvalues of a quantum mechanical system by solving the Schrödinger equation for the system – when we are able to do so. There are only a small number of systems for which we can exactly solve the Schrödinger equation, and in all other cases we have to resort to some kind of approximation or numerical method. One such method of approximation is the *Variational Method*. This method is very useful when the Hamiltonian of the system is known and we need to know the ground state energy of the system. The method is as follows.

Consider a one-dimensional system. We choose some 'trial' or 'guess' wave function for the ground state of the system, say $\psi(x, b)$, where b is the *variational parameter*. We obtain the expectation value of the Hamiltonian H with respect to this wave function $E(b) = \langle H \rangle$. This energy value is minimized with respect to the variational parameter b, and this minimum value (say $E_{\min}$) is the estimate of the ground state energy. There is a theorem, called the *Variational Principle*, which states that the variational estimate so obtained is an upper bound for the exact ground state energy, that is, $E_{\min} \geq E_g$, where E_g is the exact (often difficult to calculate) ground state energy.

The above method can be straightforwardly generalized for higher dimensional problems, and also for wave functions with several variational parameters. It can also be applied to find estimates for the excited state energies, but in practice it is usually reliable only for the ground state energy estimation. The most important part of this method is the choice of the trial wave function. It is essential that the trial wave function is consistent with the symmetry of the system. For example, if the potential energy is symmetric about a position, the ground state wave function must also be even about that point and must not have any nodes.

The following problem illustrates the method.

Problem

Consider the trial wave function

$$\psi(x) = \frac{A}{x^2 + b^2} \tag{1}$$

where A normalization constant and b is the (real) variational parameter. Use this trial wave function to estimate the ground state energy of a one dimensional linear harmonic oscillator. You can use the following integrals:

$$\int_{-\infty}^{\infty} \frac{1}{(b^2 + x^2)^2} dx = \frac{\pi}{2b^3} \tag{2}$$

$$\int_{-\infty}^{\infty} \frac{x^2}{(b^2 + x^2)^2} dx = \frac{\pi}{2b} \tag{3}$$

$$\int_{-\infty}^{\infty} \frac{x^2}{(b^2 + x^2)^4} dx = \frac{\pi}{16b^5} \tag{4}$$

Solution

Note that the given trial wave function is 'reasonable' – $\psi(x) \to 0$ for $x \to \pm\infty$, and it is even about the origin. Also it does not have any nodes.

We begin by first normalizing the wave function:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1$$
$$\Rightarrow \; |A|^2 \int_{-\infty}^{\infty} \frac{1}{(b^2 + x^2)^2} dx = 1$$
$$\Rightarrow \; |A|^2 = \frac{2b^3}{\pi}$$

In the last step we have used the integral given in stint1. Thus the normalized wave function is

$$\psi(x) = \sqrt{\frac{2b^3}{\pi}} \frac{1}{x^2 + b^2} \tag{5}$$

Harmonic oscillator Hamiltonian is

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 \tag{6}$$

where x, p, m and ω have the usual meanings. We have to find

$$E(b) = \langle \psi | H | \psi \rangle = \langle \psi | T | \psi \rangle + \langle \psi | V | \psi \rangle \tag{7}$$

where $T = \frac{p^2}{2m}$ and $V = \frac{1}{2} m\omega^2 x^2$, the kinetic and potential energy operators.

$$\begin{aligned} \langle T \rangle &= \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \left| \frac{d\psi}{dx} \right|^2 dx \\ &= \frac{\hbar^2}{2m} \frac{2b^3}{\pi} \int_{-\infty}^{\infty} \left| \frac{-2x}{(b^2 + x^2)^2} \right|^2 dx \\ &= \frac{\hbar^2}{4mb} \end{aligned} \tag{8}$$

We have used integral given in equation stint3 in the last step. Next we find $\langle V \rangle$:

$$\begin{aligned}\langle V\rangle &= \int_{-\infty}^{\infty}\psi^* V\psi dx\\ &= \frac{2b^3}{\pi}\cdot\frac{1}{2}m\omega^2\cdot\int_{-\infty}^{\infty}\frac{x^2}{(b^2+x^2)^2}dx\\ &= \frac{1}{2}m\omega^2 b^2 \qquad (9)\end{aligned}$$

In the last step here we have used integral in equation stint1. Thus we have expectation value of energy as a function of the variational parameter:

$$\begin{aligned}E(b) &= \langle H\rangle\\ &= \langle T\rangle + \langle V\rangle\\ &= \frac{\hbar^2}{4mb}+\frac{1}{2}m\omega^2 b^2 \qquad (10)\end{aligned}$$

Now we minimize $E(b)$ with respect to b:

$$\left(\frac{\partial E}{\partial b}\right)_{b=b_0} = 0$$

$$\Rightarrow \left(-\frac{\hbar^2}{2mb^3}+bm\omega^2\right)_{b=b_0} = 0$$

$$\Rightarrow -\frac{\hbar^2}{2mb_0^3}+b_0 m\omega^2 = 0$$

$$\Rightarrow b_0^4 = \frac{\hbar^2}{2m^2\omega^2}$$

$$\Rightarrow b_0^2 = \frac{\hbar}{\sqrt{2}m\omega} \qquad (11)$$

In the last step we have chosen the positive value for b_0^2, because it gives the minimum for $E(b)$, as the reader can verify by usual methods. Also, it is stated in the problem that b real. This gives us the ground state energy estimate (from equation toten) $E_{\min} = E(b_0) = \frac{\hbar\omega}{\sqrt{2}} = 0.707\hbar\omega$. This differs from the actual ground state energy of the harmonic oscillator, which as we know is $0.5\hbar\omega$, by about 40%. Note that the estimate is greater than the exact value, in agreement with the variational principle.

The above is obviously not such a good estimate. This might be improved with some other choice of the trial wave function. In fact, if we choose a Gaussian function in x, i.e., $\psi(x) = Ae^{-bx^2}$, the ground state energy estimate will be the exact the ground state energy $\frac{1}{2}\hbar\omega$ (This exercise is done in every quantum mechanics text book). This is because the trial wave function happens to be the exact ground state wave function for the harmonic oscillator .